

```
63
                                                                                65
                                                                                    66
                                                                                        75
ring nodes :
    1 2 3
               5 6 7
                         8
                            9
                               10
                                   11 12
chain bonds :
    2-37 5-38 11-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
          39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57
    38-39
    56-58 59-60 61-62 63-64 64-65 64-66
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
    2-37 5-38 11-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
exact bonds :
    14-17 15-16 16-18 19-20 21-22 21-23 39-42
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
    containing 1:7:
G1:[*1],[*2],[*3],[*4],[*5],[*6]
G2:H,CH3,Et
G3:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
                                  29:CLASS
    22:CLASS
              23:CLASS
                       28:CLASS
                                            30:CLASS
                                                      32:CLASS
                                                                33:CLASS
                                                                          34:CLASS
                                                                                    37:CLASS
    38:CLASS
              39:CLASS
                        42:CLASS
                                  44:CLASS
                                            45:CLASS
                                                      46:CLASS
                                                                47:CLASS
                                                                          48:CLASS
                                                                                    49:CLASS
```

54:CLASS

55:CLASS

56:CLASS

57:CLASS

58:CLASS

53:CLASS

50:CLASS

59:CLASS

51:CLASS

52:CLASS

```
C:\stnweb\Queries\3.str
chain nodes :
    14 15
            16
                17
                    18
                        19
                             20
                                 21
                                              28
                                                               33
                                                                                    42
                                                                                        44
                                                                                             45
```

```
46 47 48
               49 50 51
                               53
                                   54
                                       55
                                               57
                                                   58
                                                       59
                           52
                                           56
                                                           60
                                                               61
                                                                  62
                                                                      63
                                                                          64
                                                                              65
                                                                                  66
                                                                                      75
ring nodes :
    1 2 3
                       8
                           9
                              10
                                 11 12
chain bonds:
    2-37 5-38 12-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
    38-39 39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
    2-37 5-38 12-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49
    48-50 51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
exact bonds
    14-17 15-16 16-18 19-20 21-22 21-23
                                            39-42
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
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G1: [*1], [*2], [*3], [*4], [*5], [*6]
G2:H,CH3,Et
G3: [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]
```

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 12:Atom 22:CLASS 23:CLASS 28:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 34:CLASS 37:CLASS 44:CLASS 38:CLASS 39:CLASS 42:CLASS 45:CLASS 47:CLASS 46:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS

```
c:\stnweb\queries\Sb.str
```

```
chain nodes :
   14 15 16
46 47 48
               17
                  18
                      19
                          20
                                     23
                              21
                                  22
                                         28
                                             29
                                                 30
                                                     32
                                                        33
                                                            34
                                                                       39
                                                                37
                                                                    38
                                                                           42
                     51
              49 50
                          52
                              53
                                             57
                                  54
                                     55
                                         56
                                                 58
                                                     59
                                                        60
                                                            61
                                                                62
                                                                    63
                                                                       64
ring nodes :
    1 2 3
               5 6 7
                       8
                          9
                             10
                                11
                                    12
chain bonds :
    2-37 5-38 7-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
          39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57
    38-39
    56-58 59-60 61-62 63-64 64-65
                                    64-66
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
    2-37 5-38 7-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49
          51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
    48-50
exact bonds :
   14-17 15-16 16-18 19-20 21-22 21-23 39-42
normalized bonds:
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
   containing 1 : 7 :
G1:[*1],[*2],[*3],[*4],[*5],[*6]
G2:H,CH3,Et
G3:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS

30:CLASS

45:CLASS

54:CLASS

32:CLASS

46:CLASS

55:CLASS

33:CLASS

47:CLASS

56:CLASS

34:CLASS

48:CLASS

57:CLASS

37:CLASS

49:CLASS

58:CLASS

29:CLASS

44:CLASS

53:CLASS

Match level:

22:CLASS

38:CLASS

50:CLASS

59:CLASS

23:CLASS

39:CLASS

51:CLASS

28:CLASS

42:CLASS

52:CLASS

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

2.48 166.93

FILE 'REGISTRY' ENTERED AT 11:53:58 ON 12 AUG 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 AUG 2004 HIGHEST RN 725685-10-9 DICTIONARY FILE UPDATES: 11 AUG 2004 HIGHEST RN 725685-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

L5 STRUCTURE UPLOADED

=> 4 12

L5 HAS NO ANSWERS

L5 STR

=> s 15

SAMPLE SEARCH INITIATED 11:55:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

483 TO 1277

PROJECTED ANSWERS:

0 TO

L6 0 SEA SSS SAM L5

=> s 15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y
FULL SEARCH INITIATED 11:55:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 927 TO ITERATE

100.0% PROCESSED 927 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L7 0 SEA SSS FUL L5

=>

STRUCTURE UPLOADED L8

=> d 19

L8 HAS NO ANSWERS

=> s 18

SAMPLE SEARCH INITIATED 11:56:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 43 TO ITERATE

100.0% PROCESSED 43 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 467 TO 1253 PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L8 T.9

=> s 18 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 11:56:45 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 759 TO ITERATE

100.0% PROCESSED 759 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L10 0 SEA SSS FUL L8

=>

L11 STRUCTURE UPLOADED

=> d 111

L11 HAS NO ANSWERS

L11 STR

=> s l11

SAMPLE SEARCH INITIATED 11:57:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 483 TO 1277

0 TO , 0 PROJECTED ANSWERS:

0 SEA SSS SAM L11

=> s lll full

h

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: y FULL SEARCH INITIATED 11:57:46 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1024 TO ITERATE

100.0% PROCESSED 1024 ITERATIONS O ANSWERS

eb

ebc gcgb cg

SEARCH TIME: 00.00.01

L13

0 SEA SSS FUL L11

=> log y COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY 467.94 SESSION 634.87

STN INTERNATIONAL LOGOFF AT 11:58:11 ON 12 AUG 2004